

Binomial level densities

A. P. Zuker

IRES, Bât27, IN2P3-CNRS/Université Louis Pasteur BP 28, F-67037 Strasbourg Cedex 2, France
(February 9, 2008)

It is shown that nuclear level densities in a finite space are described by a continuous binomial function, determined by the first three moments of the Hamiltonian, and the dimensionality of the underlying vector space. Experimental values for ^{55}Mn , ^{56}Fe , and ^{60}Ni are very well reproduced by the binomial form, which turns out to be almost perfectly approximated by Bethe's formula with backshift. A proof is given that binomial densities reproduce the low moments of Hamiltonians of any rank: A strong form of the famous central limit result of Mon and French. Conditions under which the proof may be extended to the full spectrum are examined.

21.10.Ma,21.60.Cs,21.60.-n,27.40.+z

The vast majority of studies on level densities rely on Bethe's formula [1],

$$\rho_B(E, a, \Delta) = \frac{\sqrt{2\pi}}{12} \frac{e^{\sqrt{4a(E+\Delta)}}}{(4a)^{1/4}(E+\Delta)^{5/4}}. \quad (1)$$

Although only two parameters are involved for a given nucleus—and a third, the spin cut-off, for work at fixed angular momentum J —their dependence on mass number, excitation energy and shell effects makes their determination delicate (see [2,3] for recent work and earlier references). The problem is that the validity—and hence the success—of the formula goes well beyond the independent particle assumption made in deriving it, and one is left wondering about the true meaning of the parameters. The Shell Model Monte Carlo method provides an alternative approach to level densities [4–6] whose reliability is now established [7]. The problem is that the calculations are hard.

To combine the simplicity of Eq. (1) with a parametrization of clear microscopic origin, we propose a continuous binomial form to describe the shell model level densities. It will be shown to do well with experimental data, to reproduce strikingly Eq. (1) over a wide range of energy, and to provide a strong form of the central limit theorem (CLT), generalizing the famous result of Mon and French [8] (MF) for Hamiltonians of arbitrary rank.

Consider a system of m particles moving in D orbits, spanning a space of dimensionality d . To specify a binomial density $\rho_b(x, N, p, S)$, three parameters are needed: N , the effective number of particles, the asymmetry p , and an energy scale ε . The span (distance between lowest and highest eigenstates), centroid E_c , variance σ^2 and the adimensional energy variable x are given by

$$S = N\varepsilon, \quad E_c = Np\varepsilon, \quad \sigma^2 = Npq\varepsilon^2, \quad x = \frac{E}{S}, \quad (2)$$

Where $p + q = 1$. Calling $\bar{x} = 1 - x$, the density is

$$\rho_b(x, N, p, S) = p^{xN} q^{\bar{x}N} d \frac{\Gamma(N+1)}{\Gamma(xN+1)\Gamma(\bar{x}N+1)} \frac{N}{S}, \quad (3)$$

which reduces to a discrete binomial, $\binom{N}{n}$ if $x = n/N = n\varepsilon/S$, with integer n .

It is often convenient to introduce $\lambda = p/q$. Then

$$p^{xN} q^{\bar{x}N} d = \frac{\lambda^{xN}}{(1+\lambda)^N} d \equiv \lambda^{xN} d_0 \therefore d = d_0(1+\lambda)^N, \quad (4)$$

where d_0 is the number of states at $x = 0$. To determine N , p and S (or ε), Eqs. (2) for S and E_c cannot be used, since the spectrum is not known. We have to rely instead on the moments of the Hamiltonian \mathcal{H} , i. e., averages given by the traces of \mathcal{H}^K , to be equated with the corresponding moments of $\rho_b(x, N, p, S)$, which for low K are the same as those of the discrete binomial (Eqs. (11)). The necessary definitions and equalities follow.

$$\begin{aligned} d^{-1} \text{tr}(\mathcal{H}^K) &= \langle \mathcal{H}^K \rangle, \quad E_c = \langle \mathcal{H}^1 \rangle, \quad \mathcal{M}_K = \langle (\mathcal{H} - E_c)^K \rangle \\ \sigma^2 &= \mathcal{M}^2, \quad \overline{\mathcal{M}}_K = \frac{\mathcal{M}_K}{\sigma^K}, \quad \gamma_1 = \overline{\mathcal{M}}_3 = \frac{q-p}{\sqrt{Npq}} \\ \gamma_2 &= \overline{\mathcal{M}}_4 - 3 = \frac{1-6pq}{Npq}; \quad d = d_0(1+p/q)^N. \end{aligned} \quad (5)$$

N and p can be extracted either through the equations for γ_1 and γ_2 , or through those for γ_1 and d . The former option is unambiguous, and it has the advantage of warning us that the binomial form is doomed if $\gamma_2/\gamma_1^2 > 1$. The latter (which we adopt here) is simpler, and physically cogent for the natural choice $d_0=1$, which locates the ground state at $x = 0$. Once N and p are known, $S = (N\sigma^2/pq)^{1/2}$ follows. The centroid E_c provides the energy reference. With the simple choice, the predicted ground state is at $E_0 = -Sp$, which may not coincide with the exact value, usually taken as origin. Therefore a shift Δ may be necessary, as in Eq. (1).

Let us apply these prescriptions to ^{55}Mn , ^{56}Fe and ^{60}Ni , for which data are available [9]. There is also a Monte Carlo calculation that does very well for the first of these nuclei [5]. The space chosen by Nakada and Alhassid is the $pf + g_{9/2}$ shells. The dimensionalities are

given by $d = \binom{D}{z} \binom{D}{n}$ where $D = 30$ and z, n are the numbers of active protons and neutrons (e. g. $z = 8, n = 12$ for ^{60}Ni). In general, to proceed, we would have to calculate the three lowest moments of the Hamiltonian, a feasible task even in enormous spaces. Here we simplify matters by making first the neutral choice $p = 0.5, N = \ln d / \ln 2 = (42, 44, 49)$ for the three nuclei in the order above. Then, we bypass the calculation of σ^2 and estimate S directly. A first approximation comes from the single particle energies at $(0, 6, 7, 7, 10)$ MeV for $(f_{7/2}, p_{3/2}, f_{5/2}, p_{1/2}, g_{9/2})$ respectively, for which the differences between highest and lowest states come at $(138, 148, 170)$ MeV for $(^{55}\text{Mn}, ^{56}\text{Fe}, ^{60}\text{Ni})$. Correlations increase these numbers by an amount that ranges from 10 MeV for ^{56}Ni to 20 MeV for ^{48}Cr , according to exact calculations in the pf shell [10]. Hence the estimate $S = (153 \pm 5, 133 \pm 5, 185 \pm 5)$ for the trio. Fixing N and allowing S to vary within the error bars, the remaining uncertainty comes from the position of the ground state, which is also allowed to vary within $\pm \varepsilon/2 \approx 1.5$ MeV. Numbers that fall very comfortably within the assigned error bars: $S = (150, 165, 185), \Delta = (1.15, -0.40, 0.20)$ MeV, define binomial densities that agree very well the experimental ones [11] (where the error bars are apparently smaller than the original ones in [9]):

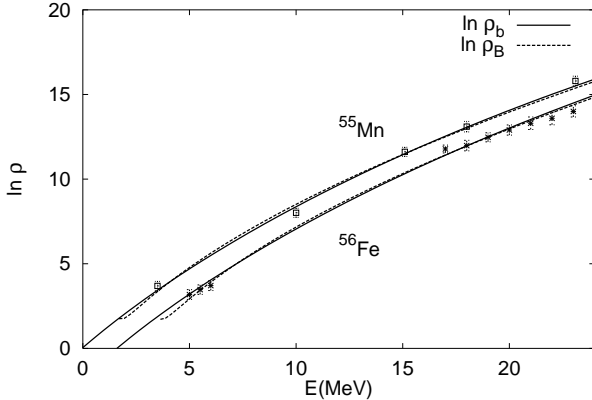


FIG. 1. Experimental, binomial (Eq. (3)) and Bethe (Eq. (1)) logarithmic level densities in ^{55}Mn and ^{56}Fe . For parameters see text.

Fig. 1 gives the experimental points for the first two nuclei, the binomials (whose parameters have been estimated above), and fits to the binomials using Bethe's formula yielding $(4a, \Delta) = (21.5, -1.5)$ and $(21.3, -3.4)$ for ^{55}Mn and ^{56}Fe respectively.

The near identity between binomial and Bethe forms extends to ≈ 40 MeV. Therefore, the immense experience accumulated by fitting Eq. (1) to the data can be reanalyzed in terms of Eq. (3) whose phenomenological potential has been illustrated by the simple exercise above. Its efficiency in dealing with rigorously calculated moments will be demonstrated in [13].

The near identity between Bethe and binomial forms has also a mathematical significance that is discussed in the paragraph that follows the one containing Eq. (15).

For ^{60}Ni in Fig. 2, instead of showing $\ln \rho_B$ —which fits obviously as well as in Fig. 1—a different check is proposed. As our finite space can provide reliable densities only in a finite interval, to have an idea of its range, the space has been enlarged by adding the $d_{3/2}$ and $s_{1/2}$ shells, at 3 MeV below $f_{7/2}$. The parameters found for the smaller space $(N, S, \Delta) = (49, 185, 0.2)$, become $(65, 285, 0.8)$ for the larger one. The densities coincide nicely in the region of interest. Discrepancies become appreciable after 25 MeV, which provides a preliminary indication: binomial densities can be trusted in an interval of $\approx 0.15S$ above the ground state. It is very much in the logic of the construction, that knowledge of the level density up to a given energy, can be extended to higher energies.

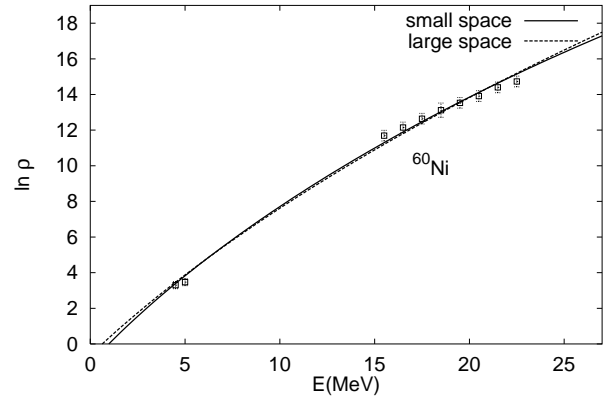


FIG. 2. Experimental logarithmic level densities for ^{60}Ni , compared with binomial ones calculated in two spaces

The first part of the program is now successfully completed.

To understand in what sense binomial and Hamiltonian moments coincide we derive the general form for both. The following notation will prove very useful (a is an arbitrary array):

$$[a]_{\neq}^l = \sum_{\alpha_1 \dots \alpha_l} a_{\alpha_1} \dots a_{\alpha_l}, \quad \alpha_i \neq \alpha_j. \quad (6)$$

If α_i can take L values, there are $L(L-1) \dots (L-l+1) \equiv L^{(l)}$ terms (Boole's notation). If the indices are ordered, $\alpha_1 < \alpha_2 < \dots$, we define analogously $[a]_{<}^l = [a]_{\neq}^l / l!$.

For the binomial case we start from the standard result

$$\mathcal{M}(t) = \sum_n p^n q^{N-n} \binom{N}{n} e^{t(n-Np)} = (pe^{qt} + qe^{-pt})^N$$

$$\mathcal{M}_K = \left(\frac{\partial}{\partial t} \right)^K \mathcal{M}(t) |_{t=0} = \mathcal{M}^{[K]} |_{t=0} \quad (7)$$

To evaluate \mathcal{M}_K , consider the multinomial expansion (Leibnitz rule) for the K -th t-derivative of a product of N factors $h_{\alpha,t}$

$$\left[\prod_{\alpha=1}^N h_{\alpha,t} \right]^{[K]} = \sum_{\alpha, k_\alpha} K! \frac{h_{1,t}^{[k_1]}}{k_1!} \frac{h_{2,t}^{[k_2]}}{k_2!} \dots = \quad (8)$$

$$\sum_{s, l_s} K! \prod \frac{[h^{[s]}]_{\leq}^{l_s}}{(s!)^{l_s}} = \sum_{s, l_s} K! \prod \frac{[h^{[s]}]_{\neq}^{l_s}}{(s!)^{l_s} l_s!}, \quad \sum_s s l_s = K.$$

In the second equality, the l_s factors with common $k_\alpha = s$ have been regrouped in $[h^{[s]}]_{\leq}^{l_s}$ and then the original ordering among the factors has been relaxed. *Notations from Eq. (6).* Note also that (obviously) $\sum_s l_s = N$.

Identifying $h_{\alpha,t} = p e^{qt} + q e^{-pt}$, we have

$$h_{\alpha,t}^{[s]} = pq [q^{s-1} e^{qt} + (-)^s p^{s-1} e^{-pt}]. \quad (9)$$

Calling $h_s = h_{\alpha,t=0}^{[s]}$ ($h_0 = 1, h_1 = 0$), and $N - l_0 = l$, the moments follow from Eq. (8), and noting that $N^{(l)} = N!/(N-l)! = N!/l_0!$, (the $N!$ coming from the equality of all the $h_{\alpha,t}$ factors), the result is:

$$\mathcal{M}_K = K! \sum_{s, l_s} N^{(l)} \prod \frac{(h_s)^{l_s}}{(s!)^{l_s} l_s!}, \quad s \geq 2. \quad (10)$$

The dominant terms maximize l , subject to the conditions $\sum s l_s = K$, $\sum l_s = l \leq N$. Keeping contributions up to $O(1/N)$, the normalized moments (\mathcal{M}_K/σ^K , $\sigma^2 = N h_2$) for $K = 2k$ and $K = 2k+1$ respectively, are

$$\frac{N^{(k)}}{N^k} (2k-1)!! \left[1 + \frac{1}{(N-k+1)} \left(\frac{k^{(2)} h_4}{6 h_2^2} + \frac{k^{(3)} h_3^2}{9 h_2^3} \right) \right],$$

$$\frac{N^{(k)}}{N^k} (2k+1)!! \frac{k h_3}{3 \sqrt{N} h_2^{3/2}}. \quad (11)$$

They will remain dominant as long as $k < \sqrt{N}$.

To calculate moments of a Hamiltonian, we write $\mathcal{H}^K = (\sum_{\alpha} h_{\alpha,t})^K$. In the single particle case $h_{\alpha,t} = m_{\alpha} \varepsilon_{\alpha}$, so the summands commute, and the multinomial expansion is **exactly** the same as in Eq. (8), with derivatives, $[s]$, replaced by powers s , and we have now $[h^s]_{\neq}^{l_s} = [\varepsilon^s m^s]_{\neq}^{l_s}$. Since $m_{\alpha}^s = m_{\alpha}$, and there are l factors, the number operators contribute as $\prod_{i=1,l} m_{\alpha_i}$, whose trace is $m^{(l)}/D^{(l)}$ (it must be proportional to $m^{(l)}$, and unity at the closed shell in which the D orbits are full). Defining $\varepsilon_{\alpha}^s = \varepsilon_{\alpha}^s D^{-1}$ the moments for a one body ($r=1$) Hamiltonian follow as

$$\mathcal{M}_K^{r=1} = K! \sum_{s, l_s} m^{(l)} \frac{D^l}{D^{(l)}} \prod \frac{[\varepsilon^s]_{\neq}^{l_s}}{(s!)^{l_s} l_s!} \quad s \geq 1. \quad (12)$$

In the dilute limit ($m \ll D$), $D^l/D^{(l)} \approx 1$, and $[\varepsilon^s]_{\neq}^{l_s} \approx (\sum_{\alpha} \varepsilon_{\alpha}^s)^{l_s} \equiv \langle \varepsilon^s \rangle^{l_s}$, the notation in MF, whose result [8,

Eq. (7)] is identical to Eq. (12) (the $s=1$ terms cancel since \mathcal{H} is taken to be traceless). The complete analogy with Eq. (10) is obvious.

To understand how to dispose of the condition $m \ll D$, let us calculate $\sigma^2(m)$, (use $\bar{m} = D - m$)

$$\langle \sum_{\alpha} \varepsilon_{\alpha}^2 m_{\alpha} + \sum_{\alpha \neq \beta} \varepsilon_{\alpha} \varepsilon_{\beta} m_{\alpha} m_{\beta} \rangle_m =$$

$$\sum_{\alpha} \varepsilon_{\alpha}^2 \left[\frac{m}{D} - \frac{m^{(2)}}{D^{(2)}} \right] = \frac{m \bar{m}}{D-1} \sum_{\alpha} \frac{\varepsilon_{\alpha}^2}{D}, \quad (13)$$

where we have added and subtracted the terms necessary to eliminate the restriction $\alpha \neq \beta$ and remembered that $\sum_{\alpha} \varepsilon_{\alpha} = 0$. Similarly, for the third moment we find

$$\mathcal{M}_3^{r=1} = \frac{m \bar{m} (\bar{m} - m)}{(D-1)^{(2)}} \sum_{\alpha} \frac{\varepsilon_{\alpha}^3}{D}. \quad (14)$$

Under particle-hole transformation (i. e. $m \rightarrow \bar{m}$), the even moments are symmetric, and the odd ones anti-symmetric, which simplifies enormously the calculations. E. g., Eq. (13) follows from the argument that $\sigma^2(m)$ must be a two body operator that reduces to the correct value for $m, \bar{m} = 1$. More generally, the leading term for $\overline{\mathcal{M}}_{2k}^{r=1} = \mathcal{M}_{2k}^{r=1}/(\sigma^2(m))^k$ must have the form

$$\frac{m^{(k)} \bar{m}^{(k)} [D^{(2)}]^k}{m^k \bar{m}^k D^{(2k)}} (2k-1)!! = \mathcal{F}(m, k) (2k-1)!!, \quad (15)$$

which follows from demanding rank $2k$, symmetry in particles and holes, vanishing for $m, \bar{m} < k$ and correct value at $m, \bar{m} = k$ (i. e. $d_k^{-1} = k!/D^{(k)}$). The important point is that $\mathcal{F}(m, k) \approx 1$ as long as $k \ll m$, i. e., *as long as this term remains dominant the moments are those of a Gaussian (CLT)*. When the leading odd moments and subdominant even ones are included we end up with an expression identical to Eq. (11) once N and p have been extracted as explained at the beginning. Hence, we have proved that the level density for a one body Hamiltonian has binomial moments for $K < \sqrt{N}$. A strong version of the central limit theorem (CLT is a statement about the even- K dominant term only).

The near identity between Eqs. (1) and (3) is an excellent reason to expect that for single particle Hamiltonians the binomial behaviour extends to the full spectrum, since Eq. (1) is a rigorous mathematical result that applies in this case.

For a Hamiltonian of higher rank, $\mathcal{H} = \sum_{xy} W_{xy} Z_x^+ Z_y$, where Z_x^+ , Z_y create and annihilate r particles, the operators do not commute. Nevertheless, Eq. (11) is of use in giving the correct counting: there are $(2k-1)!!$ ways of contracting \mathcal{H}^{2k} in k pairs, $k(2k+1)!!/3$ ways of contracting \mathcal{H}^{2k+1} in $k-1$ pairs and one triple, etc. However, the contributions of each term are different. In other words: for the dominant term, say, the factor $\mathcal{F}(m, k)$ becomes extremely complicated. The problem

was solved by Mon and French [8]. Here we give an idea of their result. For simplicity assume that \mathcal{H} is a two-body operator ($r=2$), and stay in the dilute limit. Then the variance $\sigma^2(m) = \langle \mathcal{H}^2 \rangle_m / d_m$ must be

$$\sigma^2(m) = \frac{m^{(2)}}{2} \sigma^2(2), \quad \sigma^2(2) = \frac{\sum W_{xy}^2}{d_2}, \quad (16)$$

Now consider $\langle \mathcal{H}^4 \rangle$, leading to three possible contractions, written in MF as $\mathcal{H}\mathcal{H}\mathcal{H}\mathcal{H} = AABB + ABBA + ABAB$. The first two give $m^{(2)}\sigma^2(2)^2/4 = (\sigma^2(m))^2$, but for the last one we have $m^{(4)}(\sigma^2(2))^2/4$, which vanishes at $m = 2$. The general result is that for $m = 2$ and $K = 2k$, only $t_k = \binom{2k}{k-1}/k$ terms survive, the Catalan numbers, i. e., the normalized moments of the semicircular density for Wigner's GOE ensemble. As m increases the number of surviving terms increases rapidly so as to have again $\mathcal{F}(m, k) \approx 1$.

It is straightforward to apply similar arguments to the other dominant and subdominant terms. Thus, we can combine the Mon French analysis and the advantages of the binomial geometry, to obtain a strong form of the CLT, seen to apply generally to higher rank Hamiltonians.

So far the good news. There are no bad news, but a hard question: Why stop the analysis at the low moments? As mentioned, it is practically certain that for rank one the proof of binomial behaviour must extend to the full spectrum. The strong formal analogy between rank one and higher should encourage the generalization. The catch is that, more often than not, systems undergo phase transitions. As there is little risk in attributing them to some form of collectivity, we can guess that the binomial forms will be valid in the absence of strong enough collectivity. Random Hamiltonians fulfill this condition, and I propose to include them in a larger class: *A Hamiltonian acts as random if it does not have strong enough collective components.*

There may be two reasons for the good performance of binomials in the nuclear case. One is the strong dominance of the single particle field. The other is the lack of sufficient collectivity in the nuclear Hamiltonian. It is certainly not random, as it contains sizeable pairing and quadrupole forces [12]. However, they do not seem to be strong enough. A quantitative estimate of the relative strength of the different components is given by σ^2 : we have already seen that the single particle contribution is far stronger than the two body part, and from [12]

we know that in the latter, pairing plus quadrupole only contribute a fraction of the total. Sufficient to give them a capital spectroscopic role but, apparently not the possibility of distorting the binomial forms.

The formalism is ready to examine the problem, which will become even more interesting with the suggestion that Hamiltonian matrices at fixed quantum numbers always have binomial level densities [13].

ACKNOWLEDGMENTS

Professor J. B. French provided some very early encouragements. G. Dussel insisted on the use of continuous binomials, and G. Martínez Pinedo on the use of exact continuous binomials. I had some very useful discussions with Y. Alhassid, V. K. Kota and A. Poves.

This work is dedicated to Emilia Montaner.

-
- [1] H. A. Bethe, Phys.Rev.**50**, 332 (1936).
 - [2] T. Rauscher, F. K. Thielemann and K. L. Kratz, Phys. Rev. C **56**, 1613 (1997).
 - [3] S. F. Mughabghab and C. Dunford, Phys. Rev. Lett. **81**, 4083 (1998).
 - [4] D. J. Dean, S. E. Koonin, K. Langanke, P. B. Radha, and Y. Alhassid, Phys. Rev. Lett. **74**, 2009 (1995).
 - [5] H. Nakada and Y. Alhassid, Phys. Rev. Lett. **79**, 2939 (1997), Phys. Lett. **436B**, 231 (1998).
 - [6] K. Langanke, Phys. Lett. **438B**, 235 (1998).
 - [7] Y. Alhassid, S. Liu and H. Nakada, Phys. Rev. Lett. **83**, 4265 (1999).
 - [8] K. K. Mon and J. B. French, Ann.Phys.(NY) **95**, 90 (1975).
 - [9] J. R. Huizenga, H. K. Vonach, A. A. Katsanos, A. J. Gorski and C. J. Stephan Phys. Rev. **182** (1969) 1149. A. A. Katsanos, R. W. Shaw Jr, R. Vandenbosch and D. Chamberlin Phys. Rev. C **1**, 594 (1970)
 - [10] E. Caurier, G. Martínez, F. Nowacki, A. Poves, J. Retamosa and A. P. Zuker, Phys. Rev. C **59**, 2033 (1999).
 - [11] A. S. Iljinov, M. V. Mebel, N. Bianchi, E. de Sanctis, C. Guaraldo, V. Lucherini, V. Muccifora, E. Polli, A. R. Reolon, and P. Rossi, Nucl.Phys.**A543**, 517 (1992).
 - [12] M. Dufour and A. P. Zuker, Phys. Rev. C **64**, 1641 (1996).
 - [13] next paper.